Novel Material Simulations

***Objective*: Electronic structure studies of complex ceramic materials with outstanding thermal & electrical properties.**

***Implications*: Connection of atomic-scale characteristics with engineering mechanics and elucidation of properties not available by any other method.**

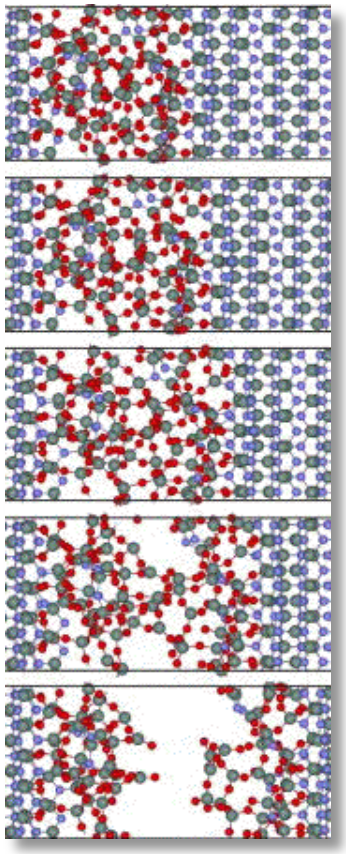
***Accomplishments:* VASP DFT study of mechanical response and failure behavior of intergranular glassy films (IGFs) in Silicon Nitrides.**

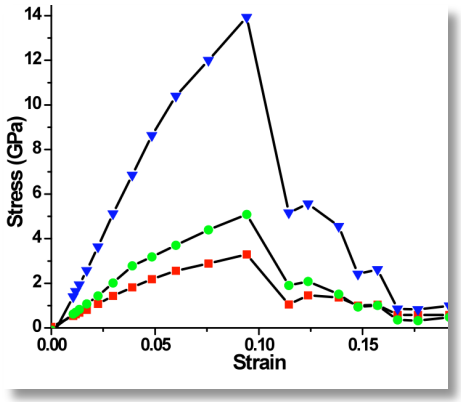
- **Stress/strain relationship explained by fundamental electronic structure of the model.**
- **May be used to guide future material designs that enhance selective properties.**

NERSC:

- **2.5M hours on Franklin used.**

PI: W. Ching, UMKC





IGF model at five different levels of strain (left) and stress vs. strain curve (right) showing a kink in the rising stress before failure, followed by a step-like post-failure behavior at higher strains.

Appl. Phys. Lett. 2009